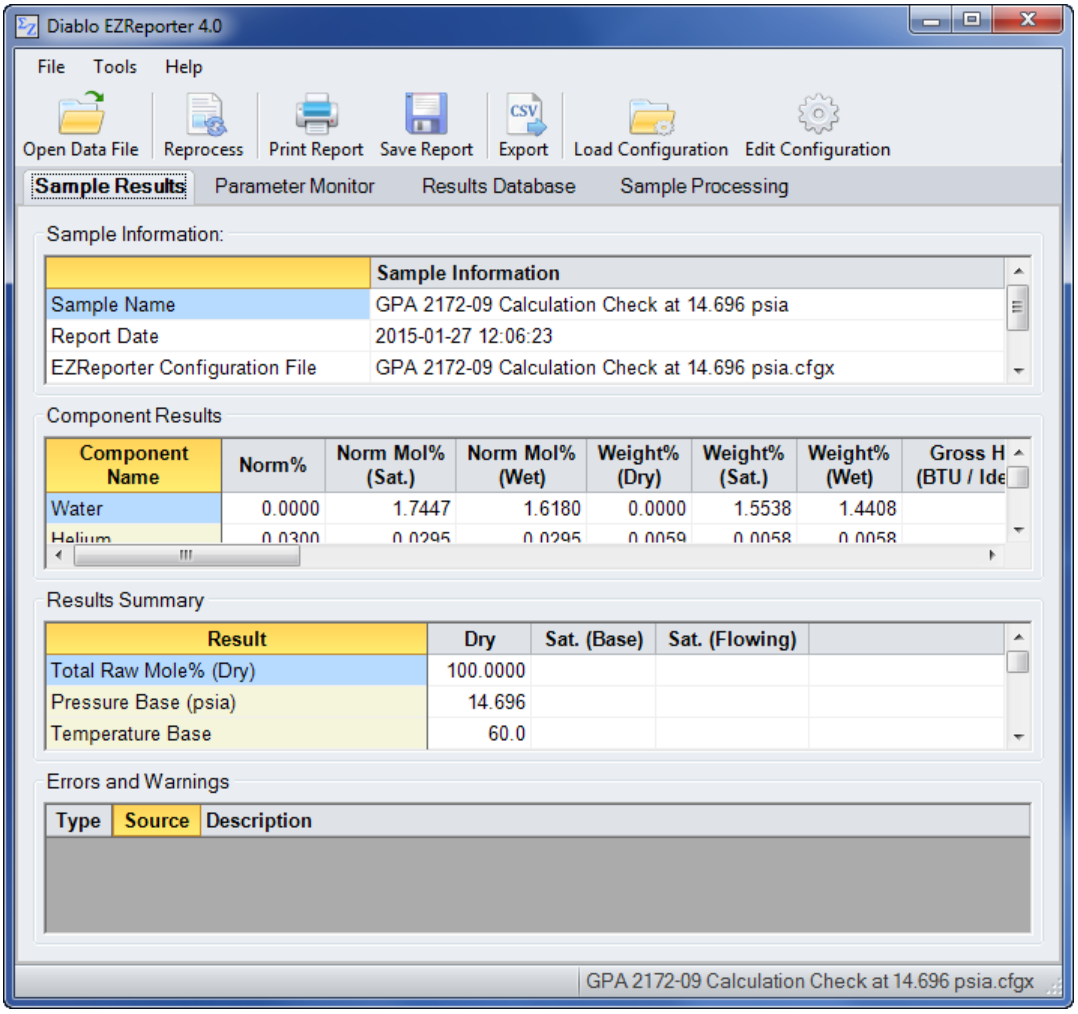
Diablo EZReporter 4.0

Agilent MSD ChemStation Connector Plugin



Diablo Analytical EZReporter Software

EZReporter 4.0 Agilent MSD ChemStation Connector Plugin

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MSD ChemStation Connector Plugin

Getting Started

This document describes how to configure the Agilent MassHunter GC/MS or MSD ChemStation chromatography data system and the EZReporter 4.0 MSD ChemStation Connector Plugin so that results can be processed automatically at the end of each run.

Supported Data Systems

The MSD ChemStation Connector plugin is intended to be used with the Agilent Technologies MSD ChemStation or MassHunter GC/MS Acquisition (single quad) data system software using MSD ChemStation Data Analysis.

Note: EZReporter does not support MassHunter Quant Data Analysis, so make sure you configure your system to use "Classic MSD ChemStation Data Analysis".

Note: A different connector plugin is required for the Agilent Technologies OpenLab GC/LC ChemStation data system.

Installation

Install the EZReporter software that includes the MSD ChemStation Connector plugin *after* installing the MSD ChemStation or MassHunter GC/MS Acquisition software. The EZReporter post-run processing macro, "ezrptx.mac", will be installed automatically to the correct ChemStation/MassHunter folder. Otherwise, the macro will be saved to the EZReporter installation folder in a ZIP file named, "ezrptx.msdchem.zip" and you will have to extract it and copy it manually to the correct folder.

Automatic Processing of MSD ChemStation Results

The Diablo EZReporter software supports automated processing of calibrated peak results generated by Agilent Technologies MSD ChemStation Data Analysis Quant reports. This support is accomplished using a post-run macro as described below.

Important: In order to process results from Agilent Technologies ChemStation Data Analysis, you must first make sure that the names in the EZReporter component settings table match the compound names in the MSD ChemStation calibration tables and Quant Report. For example, if a compound is named "Hexane" in the ChemStation calibration table, it must also be entered as "Hexane" in the component settings table (not "n-Hexane", or "nC6").

Create MSD ChemStation Quant Method

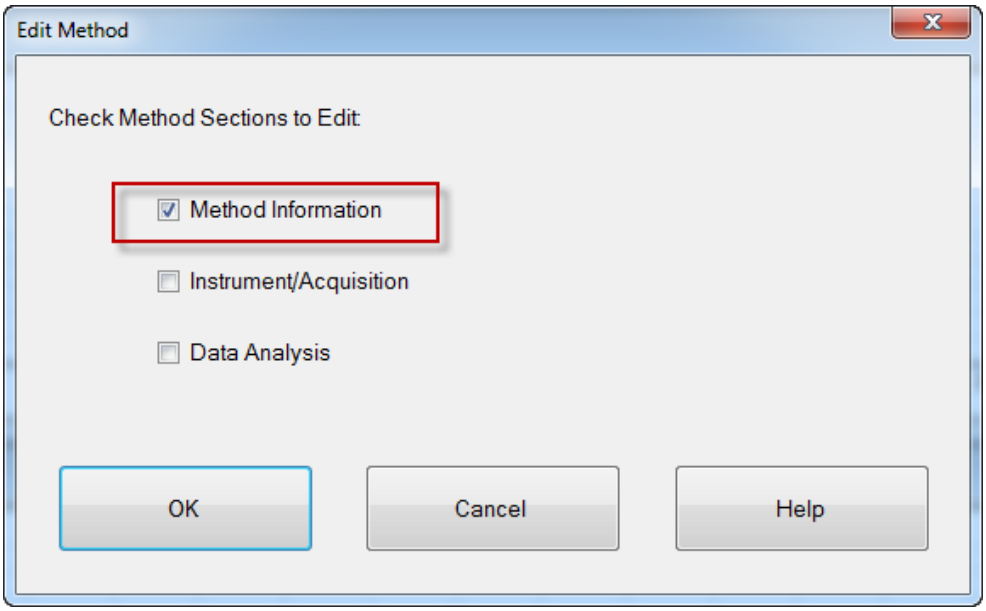
EZReporter is designed to process results from an MSD ChemStation Data Analysis Quant report. So, you must first set up quantitation, calibrate your method, and calculate a quant report before sending results to EZReporter. Please refer to the MSD ChemStation Data Analysis reference manual and help file for information.

Important: If you will be using any of EZReporter's calculated results (normalized amounts, etc.), make sure that all of the compounds are calibrated and reported using the same concentration units.

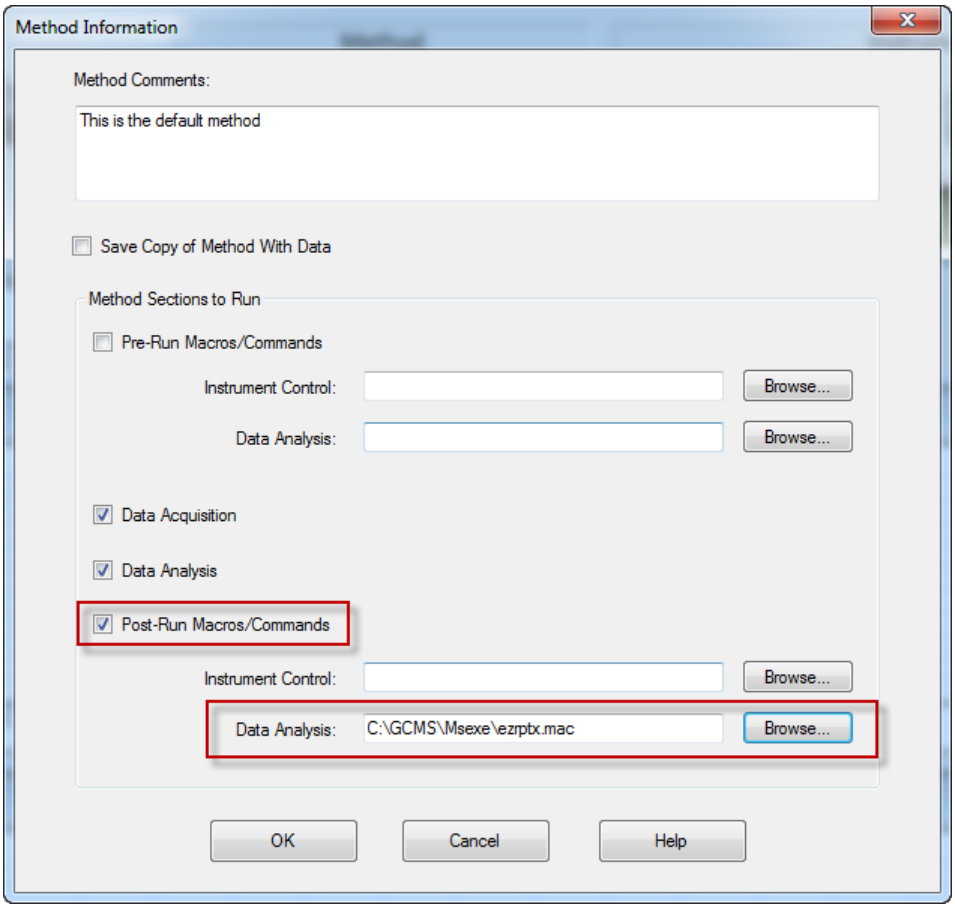
Edit the MSD ChemStation Method Information Settings

To configure an MSD ChemStation or MassHunter GC/MS method using Classic MSD ChemStation Data Analysis for automatic post-run processing with the EZReporter software, you must edit the method from the main MSD ChemStation Acquisition window (not from Data Analysis):

1. Click, "Method > Edit Entire Method" and make sure "Method Information" is checked:



2. In the Method Information window check "Post-Run Macros/Commands" and for the "Data Analysis" option, browse and select the macro "EZRPTX.MAC":



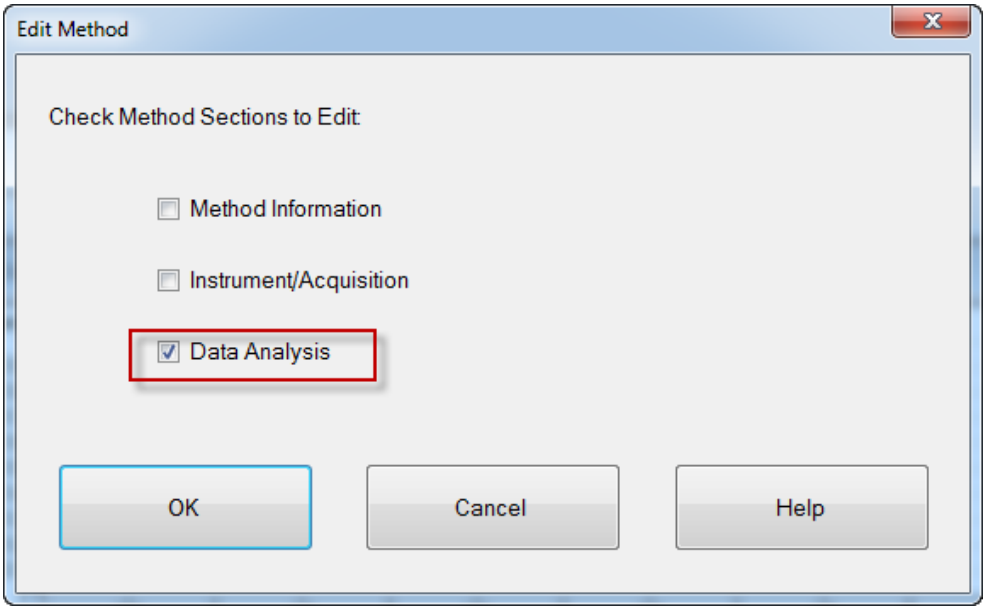
Important: Make sure to save the ChemStation method once you have made these modifications.

Note: If the EZReporter installation program detects the presence of the MSD ChemStation software on the computer, it will automatically copy the post-run macro, "ezrptx.mac" to the proper folder in the ChemStation directory structure (the "MSEXE" folder). If the ChemStation software is not detected, then the macro will be installed to the EZReporter installation folder in a ZIP file (ezrptx.msdchem.zip) and it will need to be extracted and copied manually to the ChemStation "MSEXE" folder.

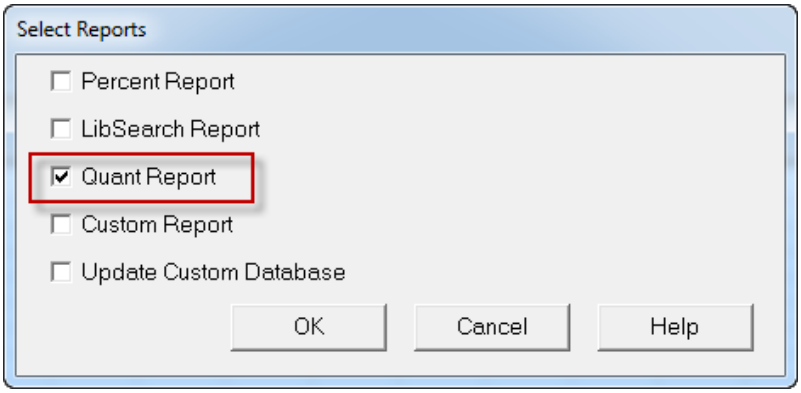
Edit the MSD ChemStation Data Analysis Settings

In order for MSD ChemStation Data Analysis "Quant" results to be processed automatically by EZReporter at the end of each run, you must also edit the method from the main MSD ChemStation Acquisition window (not from Data Analysis) and configure it to generate a "Quant Report".

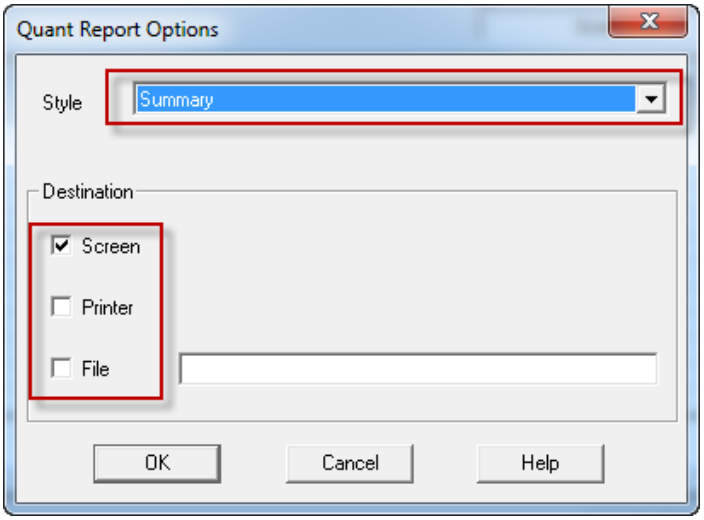
1. Click, “Method > Edit Entire Method” and make sure “Data Analysis” is checked:



2. Check “Quant Report”:



3. Select “Summary” style, and at least one of the Report Destinations must be checked:



Important: Make sure to save the ChemStation method once you have made these modifications.

Manually Re-processing MSD ChemStation Results

You can also reprocess results manually from the MSD ChemStation Data Analysis as follows:

1. Start the MSD ChemStation Data Analysis software
2. At the ChemStation command line, type the following command followed by the "Enter" key

   ```
   macro "ezrptx.mac"
   ```

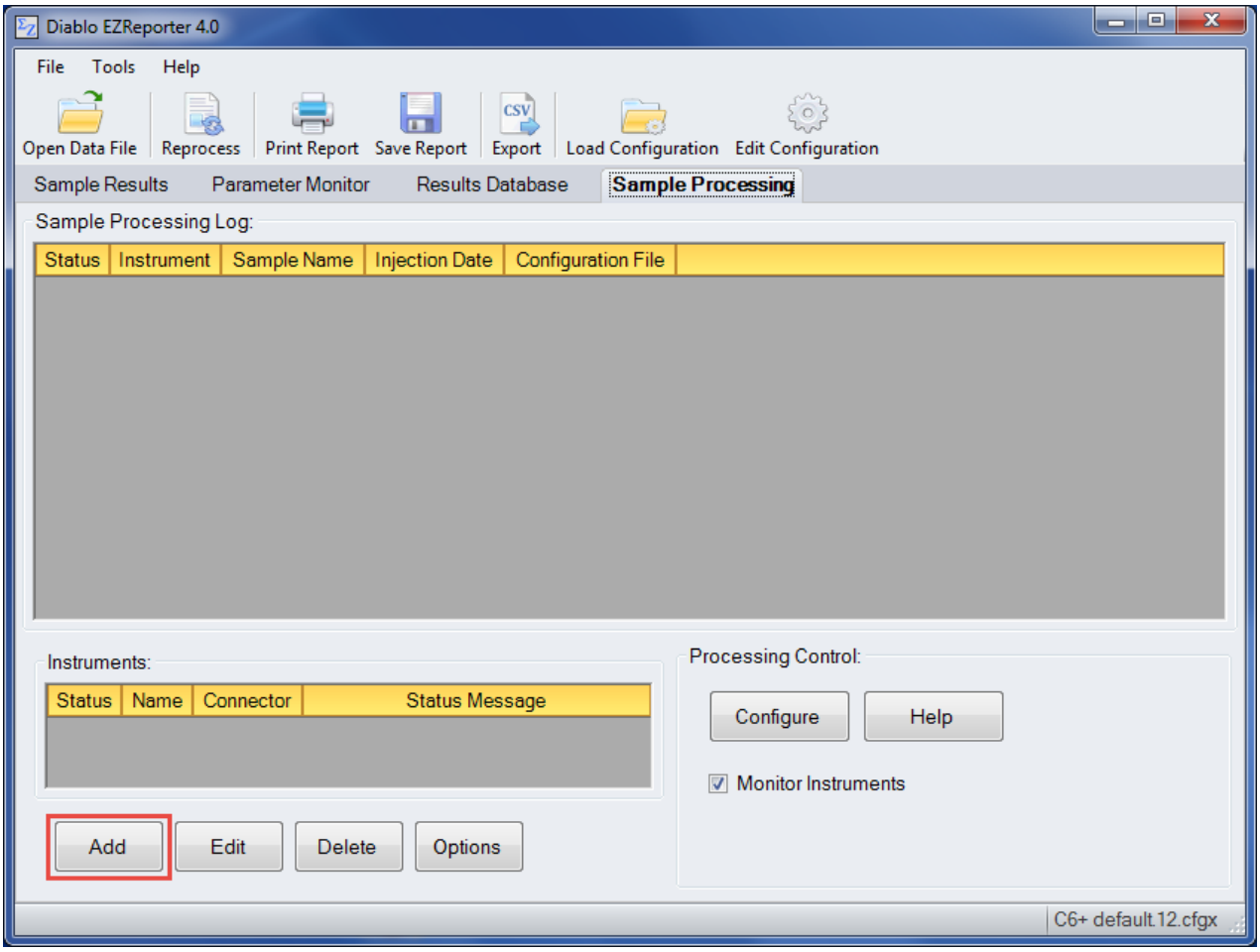
   Note: You will need to reload the macro any time you restart the ChemStation software.
3. **Important**: before sending results to EZReporter you must first make sure a Quant report has been calculated by clicking: "**Quantitate > Calculate**"
4. **Important**: Make sure that you have already started the EZReporter software before sending results.
5. From the ChemStation Data Analysis command line, enter the command, **EZReport**, to send the current results to EZReporter for processing.

Configure EZReporter

In order to process results from MSD ChemStation or MassHunter GC/MS, you must add and configure an instrument in the EZReporter "Sample Processing" tab.

Add an Instrument

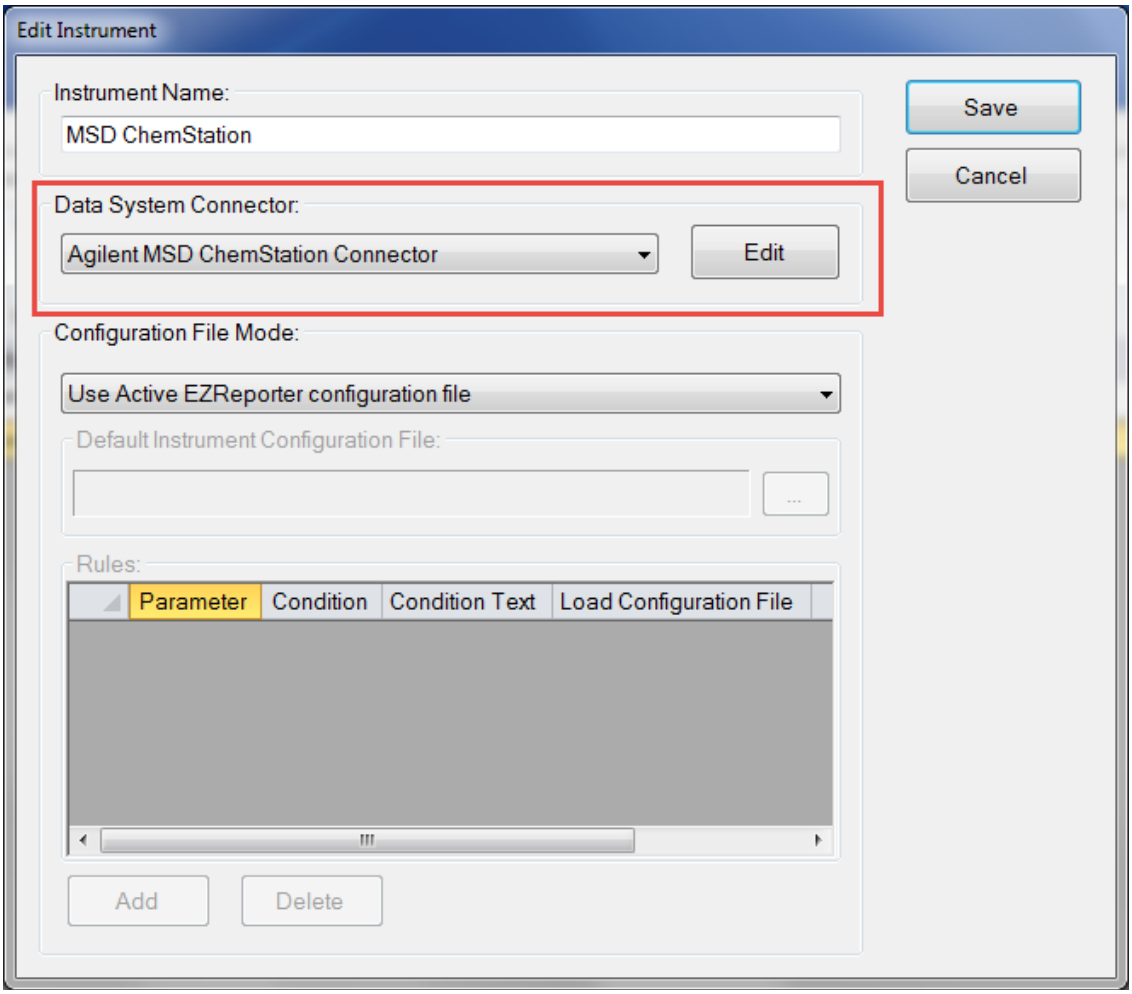
First, you must add and configure an instrument. Switch to the "Sample Processing" tab of the main window, and click the "Add" button below the instruments table.



Select the Data System Connector

In order to process results from your chromatography data system, you must select the Data System Connector for the data system you are using, and then "Edit" the connector to select and apply any connector-specific settings. Please refer to the reference manual or help file for the particular Data System Connector you are using.

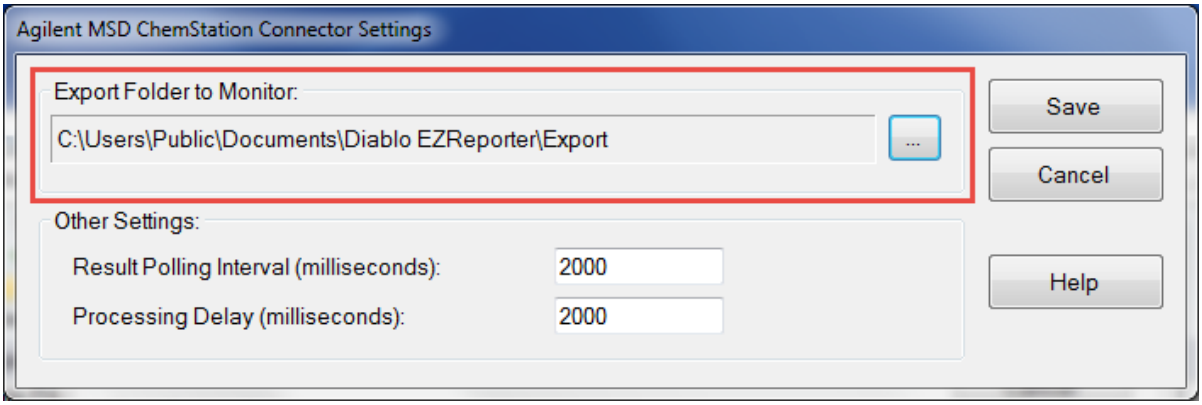
Important: The data system connectors available for you to select will be dependent on which version of the installation program you used to install the EZReporter 4.0 software. Make sure that you download the installer version for the manufacturer of the chromatography data system you are using to control your gas chromatograph.



Configure the Connector

The only setting you typically need to set for the ChemStation Connector is the "Export Folder to Monitor". Unless you are processing results from multiple instruments, you shouldn't need to change this setting from the default folder.

Important: the ezrptx.mac MSD ChemStation macro is hard-coded to use the default folder. If you change this folder, you will also need to edit the macro and change the folder.



Other Settings

These settings should not need to be changed in a typical installation.

Result Polling Interval: This is the interval in milliseconds at which the connector will check the export folder for new text files exported from ChemStation. The default value of 2000 milliseconds should be correct for most situations.

Processing Delay: After finding new text files in the export folder, the connector will wait for this period in milliseconds before processing results. The default value of 2000 milliseconds should be correct for most situations.

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